Ardra

Center for Applied Scientific Computing

Scalable Parallel Code System to Perform Neutron-and Radiation-Transport Calculations

Ardra offers robust scalable solution methods for neutron- and radiation-transport problems in complex 3D geometries. High resolution in space, energy, and direction are supported. Ardra has demonstrated its capability to solve systems with billions of unknowns on terascale computers with thousands of processors.

The ability to model the transport of neutral particles (such as neutrons and photons) through matter is important in many scientific and engineering activities. Among these are reactor and shielding design, development of medical radiation treatment, and nuclear well-logging applications, as well as others. In this work, we present a scalable, parallel code system to perform neutral particle transport calculations in three dimensions.

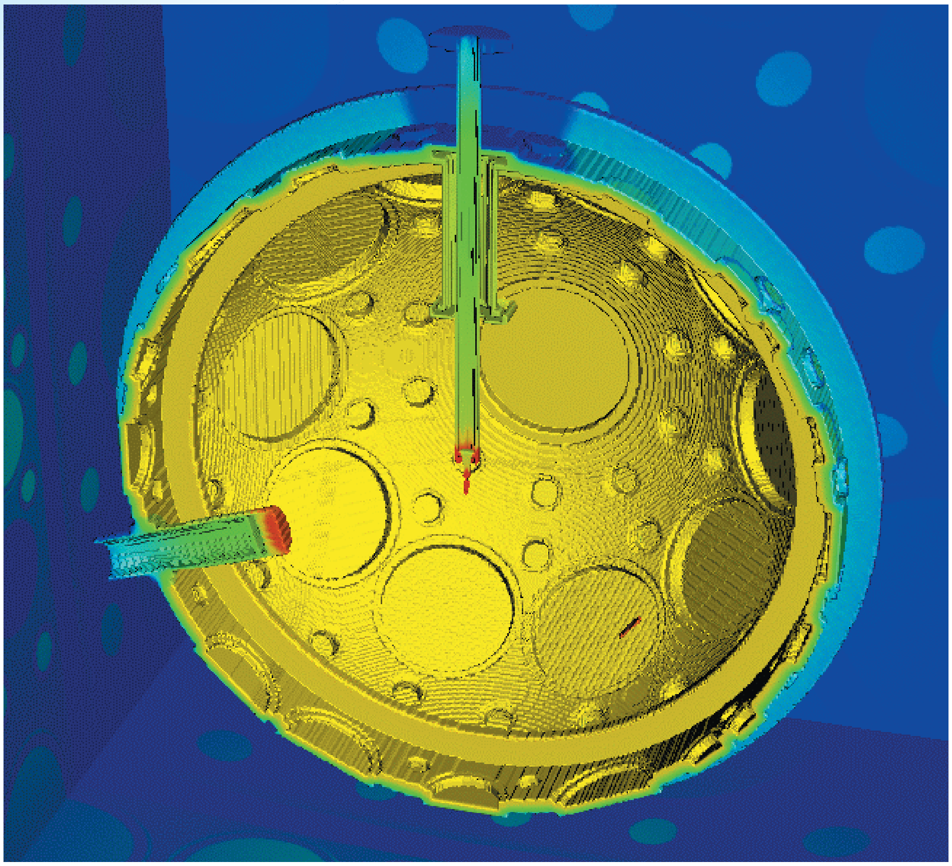

Figure 1. Isosurfaces derived from material properties display a cut-away view of the interior of the Nova target chamber. Red and blue colors on the isosurfaces represent total neutron scalar flux values at the highest and the lowest values respectively.

Overview of the Solution Method

The Ardra code exploits concurrency with respect to all phase space variables represented by direction, position and energy. The parallel execution and interprocessor communication are performed by calls to message-passing interface (MPI) library routines, which insures portability among computing platforms. Solutions to complex geometries can be obtained, as a powerful geometry package developed at Lawrence Livermore National Laboratory (LLNL) has been integrated with the code system. The geometry module produces structured Cartesian grids capable of non-uniform grid spacing. Both Dirichlet and specular reflection boundary conditions are supported. Therefore, users can take advantage of existing problem symmetries. For example, only one-eighth of a domain need be solved for problems having reflection symmetry in all three directions, a condition found in many engineering applications.

To obtain the steady state solution, either source iteration (Richardson Iteration) or a Krylov subspace method (the Biconjugate Gradient Stabilized, BiCGSTAB, algorithm) is applied in conjunction with a sweeping algorithm, to solve the discretized system. Diffusion synthetic acceleration (DSA) is implemented with a parallel semicoarsening multigrid algorithm (SMG) in a highly efficient manner, which improves the convergence behavior of the algorithm significantly in optically thick regimes.

To remedy a fundamental shortcoming of the discrete ordinates approximation, known as ray effects, a harmonic projection method has been developed and implemented within the code system. This method allows users to obtain the quality of a spherical harmonics, or P_n solution, while exploiting the efficiency and better parallelizability of the S_n method.

A Highly Efficient Solver

The SMG–DSA preconditioned BiCGSTAB solver is scalable and highly efficient. Table 1 provides performance numbers for an optically thick problem with a scattering ratio of one. Here, the problem size is scaled with the number of processors to insure a constant number of zones per processor (125,000 zones/processor). For the calculations presented in Table 1, an S_6 approximation with 48 directions is applied in

UCRL-TB-132078 Rev. 1
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Table 1. Scalability Results

Processor Topology	Iterations	Run Time (sec)
1x1x1 = 1	7	486
2x2x2 = 8	6	453
4x4x4 = 64	6	622
8x4x4 = 128	6	708

angle. For comparison, an S_2 (8 directions) calculation was performed without preconditioning on a single processor. For this calculation, the BiCGSTAB solver requires 376 iterations (738 sec), while source iteration does not converge after 15,531 iterations (4 hours).

Shielding Calculation of the Nova Target Chamber

Code capabilities are demonstrated by a shielding calculation (illustrated in Figure 1), containing more than 14 billion unknowns. To adequately resolve the spatial scale, which varies by four orders of magnitude (Figure 2), a spatial mesh of 536 x 540 x 552 mesh points (160 million zones) was selected. The neutron energy was discretized in 23 energy groups. Material properties in the calculation varied by 14 orders of magnitude.

This calculation was accomplished on the IBM ASCI Blue–Pacific computer located at LLNL. (ASCI is the national Accelerated Strategic Computing Initiative to deliver reliable terascale computing capability.) The ASCI Blue–Pacific computer manufactured by IBM is a Hypercluster of 1,464 processing nodes. The full machine consists of three 488-node sectors with a peak speed of 3.9 TFLOPS. The shielding calculation was conducted using two of the three sectors.

This calculation simulates the flux of fusion neutrons exiting the Nova laser target chamber. The neutrons are produced by the fusion of deuterium–tritium gas. To protect the experimenters from the harmful effects of the neutrons, building engineers must determine the distribution of neutron flux. They can then design the appropriate shielding structures into the building. Fusion neutrons can be very penetrating when they emerge from the target chamber because they are born at a very high energy (14.1 MeV).

Although the target chamber is packed with experimental equipment that usually absorbs the neutrons or scatters them in other directions, some directions in the target chamber lead through large voids that allow the neutrons to pass through relatively freely. It is in these directions that the high-energy neutrons can be dangerous if not absorbed in a shield. These directions show clearly in our calculations, as seen in Figure 3.

For additional information about the Ardra project, visit our web site at http://www.llnl.gov/CASC/Ardra or contact Peter N. Brown, (925) 423-2098, pnbrown@llnl.gov

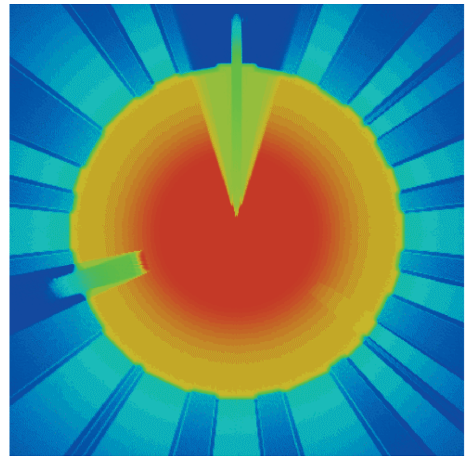

Figure 3. Total neutron scalar flux values are shown at the center plane of the Nova target chamber.

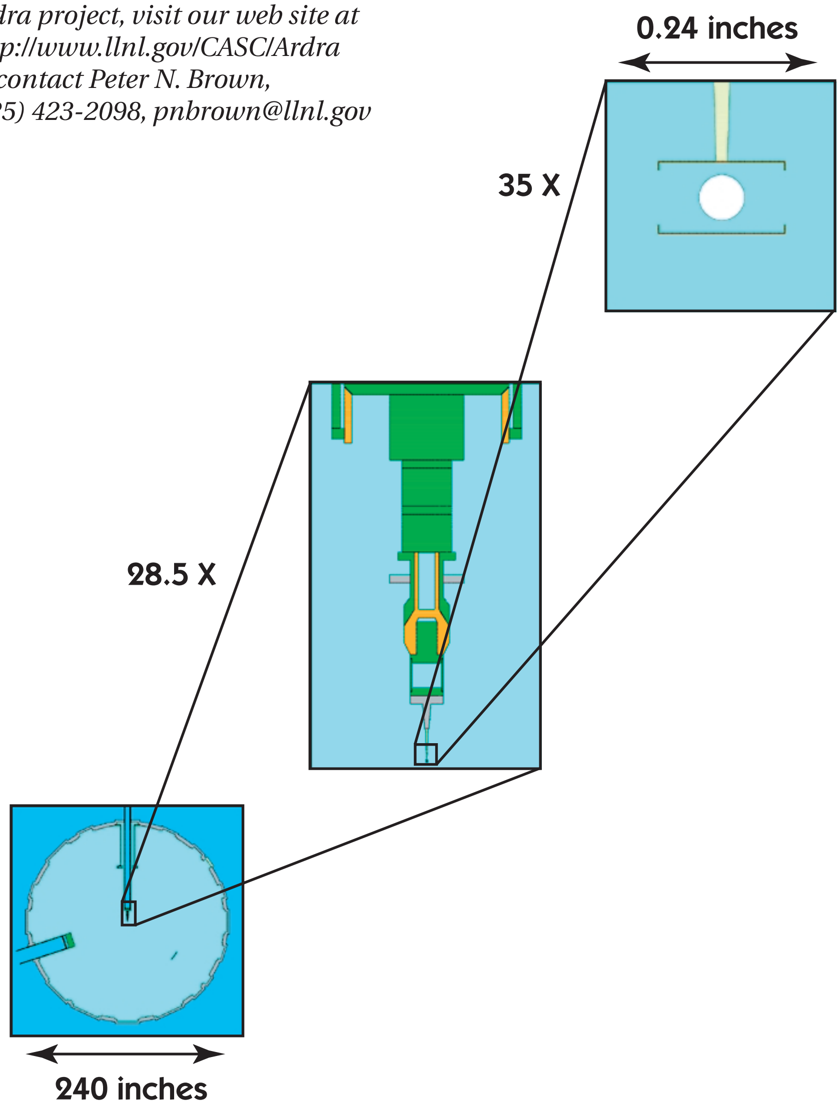

Figure 2. Significant internal structures are 1,000 times smaller than the diameter of the test chamber. A very high spatial resolution is required.

This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.